DRAFT - DETERMINING LIMITS FOR LIQUID HAZARDOUS MATERIAL - DRAFT

Abstract

This paper describes a method for calculating the volume of liquid hazardous material necessary to exceed protective action limits (e.g., Emergency Response Protective Guide-2 (ERPG-2) or the Temporary Emergency Exposure Limit-2 (TEEL-2) at 30 meters from the release point. A basic dispersion equation is used to determine the release or evaporation rate for 434 liquid chemicals found on the DOE SCAPA TEEL list, Revision 15. These release rates are used in the formulas provided with the EPIcode® and the ALOHA™ model to calculate the radius of the pool necessary to generate this rate of evaporation. The volume necessary to generate a pool with the calculated radius and one millimeter deep are presented in tables. Concentrations for selected chemicals are checked with the respective codes using a flat and an urban terrain scenario. The concentrations from the ALOHA™ model with the urban terrain scenario are approximately 6.1 greater than the ERPG-2 or TEEL-2 limits for all chemicals checked. A major difference between the models appears to be the method used to calculate the σ_y in the dispersion equation for each process. Attachments provide a listing of physical parameters for the chemicals used with this process, the calculated release or evaporation rates for those chemicals, and the volumes for flat and urban terrain scenarios necessary to generate an ERPG-2 or TEEL-2 at 30 meters from the release site.

I.   INTRODUCTION

In accordance with the Department of Energy (DOE) O 151.1 series orders, it is DOE policy to develop and maintain an emergency management system that—through emergency planning and emergency preparedness, and with effective response capabilities—is capable of responding to and mitigating the consequences resulting from emergencies. Proper emergency planning will greatly reduce the potential for loss of life and property damage, as well as increase the safety of all employees and provide protection to the environment. As part of this planning, the Department of Energy Order 151.1, paragraph V.3.a.(1)(a) states that an Alert shall be declared if "the radiation dose from any release to the environment or a concentration in air of other hazardous materials is expected to exceed … the applicable Protective Action Guide or Emergency Response Planning Guideline (ERPG) at or beyond 30 meters from the point of release to the environment…" [DOE 97]. Because LANL uses a large variety of individual chemicals, the Laboratory developed a process that calculates how much spilled-chemical inventory would cause the 30-meter criterion to be exceeded as an indication that a hazard assessment may be required. This paper outlines that process and uses standard dispersion equations for a continuous release of vapors to the environment and rapidly calculates the "acceptable" quantity of material for 434 liquid chemicals selected from the DOE SCAPA Temporary Emergency Exposure Limits (TEEL), Revision 15. This provides facility managers with a simple tool to "look up" quantities of chemicals that the facility can have "on hand" without the need to consider process flow information for emergency planning. It also provides emergency planners with a screening tool to identify when a facility exceeds quantities of material that could potentially generate a concentration above specified limits at 30 meters from the point of release and potentially require a hazard assessment.

II. METHODS

The process to develop quantities of material basically involves working the standard dispersion equation backward from the concentration at the point of interest to the amount of material released. The standard dispersion equation is long and cumbersome to work with; however, if one were interested only in a ground release along the centerline, the standard equation becomes more manageable. Based on Turner's workbook, the concentration downwind of a release is given by [EPA 87]:

$$C = Q / \pi * \sigma_y * \sigma_z * u \qquad \text{(Equation 1)}$$

where $\quad C$ = air borne concentration, g/m^3
Q = rate of release into the air, g/sec
$\sigma_y \; \sigma_z$ = dispersion deviation, horizontal (y), and vertical (z)
u = wind speed, m/sec

In working this simplified dispersion equation backwards, the desired value to calculate is the rate of release into the air. This can then be married to the evaporation rate from a particular model to determine the radius of the evaporating pool and the quantity of material released.

The airborne concentration in the above equation is set as the maximum concentration allowable before protective actions need to be taken. The ERPG-2 is the maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to one hour without experiencing or developing irreversible or other serious health effects. The Los Alamos National Laboratory has adopted the ERPG-2 as the criteria at which protective actions will be taken [EMP 98] and applies the ERPG-2 at the 30 meter point from each facility at the Laboratory as required by DOE Order 151.1. Since there are only 87 chemicals with ERPGs, the Laboratory adopted the Temporary Emergency Exposure Limits (TEELs) to expand this listing to over 1000 chemicals (Craig 99). The SCAPA-approved methodology published in the American Industrial Hygiene Journal [Craig 95] is used to obtain these hierarchy-derived TEELs. Of these chemicals with a TEEL, there are 434 liquid chemicals for which this process is applicable.

The dispersion deviations, σ_y and σ_z, can be calculated from the Briggs equations once the Pasquill stability class is determined (Briggs 1973). To simulate the worse case conditions F stability class with winds at 1 meter per second is chosen. The Briggs equations for the F stability class to estimate the σ_y and σ_z are shown in Table 1 [EPA 87].

TABLE 1: Equations Used to Estimate the Dispersion Coefficients s_y and s_z

	s_y, meters	s_z, meters
Open-Country Conditions	$0.04 * X * (1+0.0001 * X)^{-1/2}$	$0.016 * X * (1+0.0003 * X)^{-1}$
Urban Conditions	$0.11 * X * (1+0.0004 * X)^{-1/2}$	$0.08 * X * (1+0.00015 * X)^{-1/2}$

where $\quad X$ = downwind distance in meters.

These equations are only valid for distances greater than 100 m and less than 10,000 m. Using the Briggs equations for distances outside this range may introduce significant errors in the calculations. For distances less than 100 m, effects from building will change the dispersion from the facility. In some cases, this may enhance the concentration or it may diminish the concentrations at specific points. The Briggs equations can be useful in <u>only</u> estimating the dispersion deviations, σ_y (est.) and σ_z (est.). Since this process is only providing a screening tool, it is believed that an estimate of the dispersion deviations is good enough. For distances less than 100 m for which there is a real need to know the approximate concentration, other methods should be considered.

These equations along with Equation 1 were used in an Excel Spreadsheet that contained the chemicals listed in "ERPGs and TEELs for Chemicals of Concern, Rev 15 Abbreviated" (WSMS-SAE-98-00101) [Craig 99].

It was not the intention of this process to review or change the physical parameters listed in Table 1 of the ERPG/TEEL document, however, because the vapor pressure is an important parameter in this process, many of the chemicals were reviewed and changes made where necessary. The following method was used to provide missing data to the table:

- If the vapor pressure was already present in Table 1 of the TEEL document, there were no changes made for that chemical in the table.
- If the vapor pressure was missing in Table 1 but could be found in a Material Safety Data Sheet (MSDS) from a manufacturer or from other government agencies (both domestics and foreign), it was entered into the physical data for the chemical in question (see Attachment 1).
- The physical properties for that chemical were reviewed and changed, as necessary, to reflect the MSDS maintained in Emergency Management.
- All changed data were highlighted for quick review (see Attachment 1).

The standard temperature selected for the chemical and the surroundings was selected to be 20 ^{o}C, but the vapor pressure for many substances is not available at this temperature. Vapor pressure varies over a range of temperatures. In some cases, this variation approximates an exponential equation and in other cases (especially where the temperature differences are small) this variation approaches a linear relationship. If the parameters are available, the Antoine equation or a similar approximation should be used to approximate the vapor pressure for substance. Since Antoine parameters could not be located for all the chemicals listed in the TEEL document, the vapor pressure at 20 ^{o}C was estimated using a linear ratio (e.g., (VP @ 25 C / 25)* 20 = VP @ 20 C). This estimate introduces errors into the estimated release rates that should be evaluated at a later date. For this exercise, the linear relationship is assumed.

Because some chemicals have a relatively high vapor pressure at environmental temperatures, a correction to the evaporation rate is recommended. The given evaporation rate should be multiplied by the correction factor as calculated below. Normally this correction factor is approximately 1.0 but this will increase as the vapor pressure of the chemical increases [Evans et al]:

$$C = - (Pa / VP) * Ln(1- VP/Pa)$$

where   C = correction factor for volatility
                           Pa = atmospheric pressure (Pascal) [101,325 Pa at sea level]
                           VP = vapor pressure of the component of concern (Pascal)

The evaporation rate corrected for volatility are presented in Attachment 3 and Attachment 4. The uncorrected evaporation rate for each chemical is presented in Attachment 2.

For some liquids, the specific gravity or density is given as a range of numbers. To estimate a number that could be used in calculations, the average between these two numbers is used. If the specific gravity or density is given by a source at a temperature different from 20 ^{o}C, a similar process as described for estimating the vapor pressure is used to estimate the specific gravity or density of a substance. This also introduces errors into the calculations that need to be considered at a later date.

The following conservative assumptions are made for the modeling effort;

- The terrain is either flat or has an urban (or roughness) component (this assumption changes which σ_y and σ_z values are used in the calculations).
- All chemicals are released from ground level.
- F Stability and 1 meter per second wind speed, representing stable air and low wind speed conditions.
- All releases are term releases (i.e., evaporation is complete after a specified time).
- Once the liquid evaporates, there is no phase change in the plume.
- The plume and chemical pool are at ambient temperature.
- The released chemical is neutrally buoyant in air.
- Only concentrations along the centerline of the plume are of interest.
- The release chemical has a Gaussian distribution in its horizontal and vertical planes.
- Liquids are instantaneously spilled onto a flat, smooth surface for a 1-mm deep circular pool and are allowed to evaporate at ambient conditions.
- The rate of release is assumed to be the evaporation rate (rate of volatilization) for spilled chemicals.

Manipulating Equation 1, the rate of release to produce the concentration of concern at 30 meters from the release source can be calculated. This rate of release can then be used in various models to determine a release radius.

Using the EPIcode[â] Model

EPIcode[®] and the EPA "Green Book" (Technical Guidance for Hazards Analysis) uses the Clement's methodology for calculating the evaporation rate for a liquid pool [Homann 96 and EPA 87]. After combining terms, the basic equation can be written as [Homann 96]:

$$Q = 0.0139 * u^{7/9} * MW^{2/3} * A * VP(T1) / T1(^{o}K) \qquad \text{(Equation 2)}$$

where
Q = rate of release in air (lbs./min)
u = wind speed (m/sec)
MW = molecular weight (g/mole)
A = surface area of spilled material (meter^2) = $\pi * r^2$
$VP(T1)$ = vapor pressure of material at temperature T1 (mm Hg)
$T1(^{o}K)$ = Temperature of spilled material (^{o}K)

Solving Equation 2 for the area, the radius of the spilled material can be calculated and by using the estimated specific gravity or density of the material, the quantity of the material can be determined.

Using the ALOHAä Model

Using the paper "Modeling Hydrochloric Acid Evaporation in ALOHA™" (Report No. HAZMAT 93-3) [Evans et al], a similar process as described above was used. The report uses four equations to calculate the evaporation rate, the mass transfer coefficient, the Schmidt number, and the molecular diffusivity of a chemical. The rate of release is determined in the same manner as stated above. The Schmidt number and the molecular diffusivity are not dependent upon the amount of released material present.

The Schmidt number is calculated as follows [Evans et al]:

$$Sc = \nu / D_m$$

where
Sc = the laminar Schmidt number for the material of interest.
ν = the kinematic viscosity of air (ALOHA™ value = 1.5 E-5 m^2/sec).
Dm = the molecular diffusivity of the material of interest in air (m^2/sec)

ALOHA™ uses Graham's Law to approximate the molecular diffusivity of a chemical as follows [Evans et al]:

$$Dm = D_{H2O} * (MW_{H2O} / MW_m)^{\frac{1}{2}}$$

where
Dm = the molecular diffusivity of the material of interest (m^2/sec).
D_{H2O} = the molecular diffusivity of water (2.4 E-5 m^2/sec at 8 ^{o}C).
MW_{H2O} = the molecular weight of water (18 kg/kmol).
MW_m = the molecular weight of the material of interest (kg/kmol)

The evaporation rate is calculated as follows [Evans et al]:

$$E = A * K_M * (MW_m * PV / R * T)$$

where
E = evaporation rate (kg/sec).
A = area of the evaporating puddle (m^2).
K_M = mass transfer coefficient (m/sec).

MW_m = molecular weight of the material of interest (kg/kmol).
PV = vapor pressure (Pa).
R = the gas constant (8314 J/kmol ^{o}K).
T = ambient temperature (^{o}K) [20 ^{o}C = 293.2 ^{o}K].

ALOHA™ uses the following equation to calculate the mass transfer coefficient [Evans et al]:

$$K_M = 0.0048 * U^{7/9} * Z^{-1/9} * Sc^{-2/3}$$

where
K_M = mass transfer coefficient (m/sec).
U = wind speed (m/sec) [worse case = 1 m/sec].
Z = the pool diameter in the along-wind direction (m).
Sc = the laminar Schmidt number.

Both the evaporation equation and the mass transfer coefficient equations are a function of the pool radius (i.e., A(area) = $\pi * r^2$ and Z (diameter) = 2r). Placing the mass transfer coefficient into the evaporation equation and solving for the pool radius (r), provides the following equation:

$$X = r^{17/9} = (0.225 * K_M * R * T * Sc^{2/3}) / (\pi * MW * PV * U^{7/9}), \text{ and}$$

$$r = 10^{((\log (X)) / (17/9))}$$

where
r = pool radius (m)
(all other terms have been previously defined)

Once the pool radius and the depth of the pool is determined (i.e., 1 mm), the volume of the resulting spill can be determined. This volume indicates the possible need for a hazard assessment and if that volume is spilled an "Alert" for a hazardous material operational emergency must be declared [DOE 97].

III.   RESULTS AND DISCUSSION

Using the above equations as a basis, the critical factors in each of the calculation methods are the physical data, especially the vapor pressure. The TEEL tables [Craig 99] provided the physical data for over 1000 chemicals, but some of the data were found to be lacking for a number of chemicals. Attachment 1 lists the chemicals found in the TEEL Table 1 and includes changes to that table. Where the vapor pressure was missing from the TEEL table for a chemical, the Internet was searched and new vapor pressure datum was placed in the table with the source for the information listed under the 'Comments' column of Attachment 1. A hardcopy of the information was obtained and the other physical data were changed as appropriate for the source listed.

Attachment 2 provides a side-by-side comparison of the release rate (based on Equation 1 above), not corrected for volatility, for both a flat terrain and an urban terrain scenario for the liquid chemicals listed in Attachment 1. It also converts the TEEL value to mg/m^3 using the conversion factors listed in the TEEL tables [Craig 99] and estimates the vapor pressure at 20 ^{o}C

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based on a linear relationship as described above. This estimate for the vapor pressure is extremely crude and may introduce substantial errors into this process. However, for some chemicals this approximation is fairly close to that observed. For example, looking at hydrogen cyanide (HCN), a Laboratory Chemical Safety Summary by the National Academy of Science and the Howard Hughes Medical Institute lists its vapor pressure as 750 mm Hg @ 25 ^{o}C [Lab Safety]. Converting this value with the linear process described above provides an estimated vapor pressure of 600 mmHg @ 20 ^{o}C. The model used at Los Alamos National Laboratory, MIDAS, lists the vapor pressure for HCN as 606 mmHg @ 20 ^{o}C. At least for this chemical, there is close agreement between the "estimated" vapor pressure and the value used by the MIDAS model.

Attachment 3 and Attachment 4 provides quantity limits established for urban and flat terrain dispersion, respectively. As can be seen the quantity of material calculated for the EPIcode$^®$ and the ALOHA™ methodologies are different by a factor less than four for the urban terrain and less than a factor of 6.3 for the flat terrain. According to published reports, the ALOHA™ Gaussian model is at least 40% more conservative than results measured for the Project Prairie Grass and generally are greater at shorter distances [ALOHA™ QA]. Since the above methodology started with a set concentration limit (i.e., the TEEL-2 for a given substance) and worked the problem backwards to obtain a radius for the released chemical, the net result of this conservatism would show up as a lower value. With the errors introduced throughout this process, being off by these relatively small factors shows fairly good agreement between the two methods.

To check the resultant values from the EPIcode$^®$ method, the EPIcode$^®$ model was run as a term release using the evaporation time and the calculated EPI quantity. Similar assumptions were made for these check calculations as used in developing the methodology (i.e., assume a ground release with F Class stability and 1 m/s wind speed using an urban terrain dispersion). Table 2 and Table 3 lists the results of these calculations for urban terrain and flat terrain, respectively. The percentage difference between the TEEL-2 limits and the concentrations calculated using EPIcode$^®$ were either zero or negative. It is believed that these differences relate to the rounding of numbers, between the calculated values and EPIcode$^®$. There is a less than 7% difference between the quantities calculated using the above-described method and the results from EPIcode$^®$.

To check the resultant values from the ALOHA™ method, the ALOHA™ model was run as a direct release using the release rate as calculated from the basic dispersion equation (equation 1). Table 4 and Table 5 lists the results of these calculations for flat terrain and urban terrain, respectively. The percentage difference between the TEEL-2 limits and the concentrations calculated using the ALOHA™ model were less than 0.3% for the flat terrain scenario and can be attributed to rounding errors. The radius of the chemical release was checked by plugging the calculated radius back into the equations listed under the ALOHA™ method. All the resulting evaporation rates compared well with the release rates calculated using the basic dispersion equation.

Since LANL has rough terrain, a similar check was performed for the urban mode in ALOHA™. When release rates calculated using the basic dispersion equation (equation 1) and the calculated σ_y and σ_z for urban terrain (Table 1) were plugged into ALOHA™ model, the resulting

concentrations were approximately 6.1 times larger than the desired TEEL-2 values (see Table 4). There are several differences between the ALOHA™ model and the method used in this paper. ALOHA™ uses a different methodology to calculate the σ_y for urban terrain than used by EPIcode® [Homann 96] and EPA guidance [EPA 87]. ALOHA™ uses a different method in calculating a release from a pool of liquid, limits the release times to less than 60 minutes and requires the pool depth to be greater than 5mm.

The Laboratory utilizes the MIDAS model to determine the level of response to an emergency (e.g., protective actions, potential exposure to personnel, etc.). To determine which of the above methods provides the better quantity for use at Los Alamos, the MIDAS model was run using similar assumptions as used in these methodologies. Looking at hydrogen cyanide, there is good agreement between the MIDAS model and the ALOHA™ methodology when MIDAS is run in the heavy gas mode, and there is good agreement between the MIDAS model and the EPIcode® methodology when MIDAS is not run in the heavy gas mode. Thus, the vapor density of the individual chemical will play an important role in determining whether to choose the EPIcode® quantity or the ALOHA™ quantity at Los Alamos National Laboratory.

SUMMARY AND CONCLUSIONS

The "backwards" calculation processes presented in this paper allows one to establish quantities of released materials that may exceed established criteria at 30 meters from the point of release. It assumes a ground release scenario in the open environment with worst weather conditions (i.e., F Class stability and 1 m/s wind speed) using urban terrain and flat terrain dispersion coefficients and does not model the release as an evaporative pool.

There are differences between the results obtained using the EPIcode® and the ALOHA™ models. The use of the EPIcode® and the ALOHA™ model was not extensive and one should not attempt to draw any conclusions from the data presented in this paper. In general, the EPIcode® provides results that are a factor of 5 lower than ALOHA™ model using an urban terrain and a factor of 6.3 higher than the ALOHA™ model using a flat terrain. Checking the results by using the calculated values in the respective models provided good agreement with the ERPG or TEEL criteria using the EPIcode® with either scenario and using the ALOHA™ model with the flat terrain. This was not the case using the ALOHA™ model and the default urban terrain setting. The ALOHA™ modeled values are 6.1 times higher than the ERPG or TEEL criteria. These differences result in the way the dispersion coefficient, σ_y, is calculated between the process presented here and the ALOHA™ model. Different methods can be used to determine the quantity of material necessary to "reach out and touch the neighbors" and should also be investigated before one establishes criteria for a chemical user.

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TABLE 2: **Comparison of the TEEL-2 Limits with the Concentrations Calculated by EPIcode[a] using the Calculated Evaporation Time and Quantity and Urban Terrain for Selected Chemicals.**

Chemical Name	CAS Number	Uncorrected Evaporation Rate @ 20 ^{o}C (g/s)	Calculated Evaporation Time (min)	Calculated Quantity (bs..)	Conc via EPIcode[a] (mg/m^3)	TEEL-2 Limits (mg/m^3)	% Diff
Acetic Acid	64-19-7	2.12	280	79	85	86.1	-1.3
Benzyl Chloride	100-44-7	1.28	2250	380	51	51.7	-1.4
Cyclohexane	110-82-7	110	57	860	4400	4472	-1.6
Chloroform	67-66-3	6.02	18	16	240	244	-1.6
o-Dichlorobenzene	95-50-1	7.42	2180	2135	300	300.5	-0.2
Diketene	674-82-8	0.424	320	18	17.0	17.2	-1.2
Ethyl Acetate	141-78-6	178	28	665	7200	7200	0.0
Ethylene Glycol	107-21-1	2.51	65870	21850	100	101.6	-1.6
Formaldehyde	50-00-0	0.304	106	4.4	12	12.3	-2.4
Hydrazine	302-01-2	0.026	506	1.7	1	1.048	-4.6
Isobutyl Alcohol	78-83-1	18.7	234	580	750	757.5	-1.0
Malathion	121-75-5	1.23	4.5×10^7	7.3×10^6	49	50	-2.0
Mercury	7439-97-6	0.00247	1×10^7	3300	0.1	0.1	0.0
Methyl Isocynate	624-83-9	0.0287	8.6	0.042	1.1	1.165	-5.5
Nitric Acid (>70%)	7697-37-2	0.955	90	12	38	38.7	-1.8
Nitroglycerin	55-63-0	0.0494	12650	83	2.0	2.0	0.0
Perchloroethylene	127-18-4	33.5	180	793	1300	1356	-4.1
Propionic Acid	79-09-4	1.12	520	78	45	45.45	-1.0
Toluene	108-88-3	27.9	90	330	1100	1131	-2.7
Xylene	1330-20-7	21.4	226	641	860	868	-0.9

Note: Numbers for the evaporation time and quantity are for the uncorrected evaporation rates.

TABLE 3: **Comparison of the TEEL-2 Limits with the Concentrations Calculated by EPIcode$^{®}$ using the Calculated Evaporation Time and Quantity and Flat Terrain for Selected Chemicals**

Chemical Name	CAS Number	Uncorrected Evaporation Rate @ 20 ^{o}C (g/s)	Calculated Evaporation Time (min)	Calculated Quantity (lbs.)	Conc via EPIcode[a] (mg/m^3)	TEEL-2 Limits (mg/m^3)	% Diff
Acetic Acid	64-19-7	0.154	278	5.7	81	86.1	-5.9
Benzyl Chloride	100-44-7	0.0926	2250	28	49	51.7	-5.2
Cyclohexane	110-82-7	8.01	57.4	61	4200	4472	-6.1
Chloroform	67-66-3	0.440	17.7	1.1	230	244	-5.7
o-Dichlorobenzene	95-50-1	0.538	2180	160	280	300.5	-6.8
Diketene	674-82-8	0.0308	320	1.3	16	17.2	-7.0
Ethyl Acetate	141-78-6	12.9	28.3	51	6800	7200	-5.6
Ethylene Glycol	107-21-1	0.182	65900	1600	96	101.6	-5.5
Formaldehyde	50-00-0	0.022	106	0.32	12	12.3	-2.4
Hydrazine	302-01-2	0.00188	506	0.13	1.0	1.048	-4.5
Isobutyl Alcohol	78-83-1	1.36	234	42	710	757.5	-6.2
Malathion	121-75-5	0.0895	4.50×10^7	5.3×10^5	47	50	-6.0
Mercury	7439-97-6	0.000179	1.02×10^7	240	0.094	0.1	-6.0
Methyl Isocynate	624-83-9	0.00209	8.61	0.0032	1.1	1.165	-5.6
Nitric Acid (>70%)	7697-37-2	0.0693	90.3	0.86	37	38.7	-4.3
Nitroglycerin	55-63-0	0.00358	12700	6.0	1.9	2.0	-5.0
Perchloroethylene	127-18-4	2.43	179	58	1300	1356	-4.1
Propionic Acid	79-09-4	0.0814	521	5.6	43	45.5	-5.5
Toluene	108-88-3	2.03	90.1	24	1100	1131	-2.7
Xylene	1330-20-7	1.55	226	47	820	868	-5.5

Note: Numbers for the evaporation time and quantity are for the uncorrected evaporation rates.

TABLE 4: **Comparison of the TEEL-2 Limits with the Concentrations Calculated by ALOHAä using the Direct Release Mode and Flat Terrain for Selected Chemicals**

Chemical Name	CAS Number	Uncorrected Evaporation Rate @ 20 °C (g/s)	Calculated Evaporation Time (min)	Calculated Quantity (lbs.)	Conc via ALOHAä (mg/m³)	TEEL-2 Limits (mg/m³)	% Diff
Acetic Acid	64-19-7	0.154	107	2.2	86	86.1	-0.1
Benzyl Chloride	100-44-7	0.0926	950	12	51.7	51.7	0.0
Cyclohexane	110-82-7	8.01	26	27	4470	4472	-0.04
Chloroform	67-66-3	0.440	6.1	0.4	244	244	0.0
o-Dichlorobenzene	95-50-1	0.538	1007	72	300	300.5	-0.2
Diketene	674-82-8	0.0308	113	0.46	17.2	17.2	0.0
Ethyl Acetate	141-78-6	12.9	13	22	7200	7200	0.0
Ethylene Glycol	107-21-1	0.182	35300	850	NL	101.6	--
Formaldehyde	50-00-0	0.022	34	0.1	NL	12.3	--
Hydrazine	302-01-2	0.00188	160	0.040	1.05	1.048	+0.2
Isobutyl Alcohol	78-83-1	1.36	103	19	759	757.5	+0.2
Malathion	121-75-5	0.0895	3.4×10^7	4.0×10^5	NL	50	--
Mercury	7439-97-6	0.000179	4.2×10^6	100	NL	0.1	--
Methyl Isocynate	624-83-9	0.00209	2.2	0.0008	1.17	1.17	0.0
Nitric Acid (>70%)	7697-37-2	0.0693	31	0.29	38.7	38.7	0.0
Nitroglycerin	55-63-0	0.00358	4800	2.3	NL	2.0	--
Perchloroethylene	127-18-4	2.43	77	25	1360	1356	+0.3
Propionic Acid	79-09-4	0.0814	202	2.2	45.5	45.5	0.0
Toluene	108-88-3	2.03	38	10	1130	1131	0.0
Xylene	1330-20-7	1.55	100	21	866	868	-0.2

Note: Numbers for the evaporation time and quantity are rounded. Actual numbers used in determining the difference can be found in the appendices.

NL = Not Listed   NR = Not run (volume too small or parameters not in model)

TABLE 5: Comparison of the TEEL-2 Limits with the Concentrations Calculated by ALOHA™ using the Direct Release Mode and Urban Terrain for Selected Chemicals

Chemical Name	CAS Number	Uncorrected Evaporation Rate @ 20 °C (g/s)	Calculated Evaporation Time (min)	Calculated Quantity (lbs.)	Conc via ALOHAä (mg/m^3)	TEEL-2 Limits (mg/m^3)	% Diff
Acetic Acid	64-19-7	2.12	125	35	523	86.1	+610
Benzyl Chloride	100-44-7	1.28	110	190	316	51.7	+610
Cyclohexane	110-82-7	110	30	450	27200	4472	+610
Chloroform	67-66-3	6.02	7.1	6.4	1488	244	+610
o-Dichlorobenzene	95-50-1	7.42	1200	1200	1830	300.5	+610
Diketene	674-82-8	0.424	132	7.4	105	17.2	+610
Ethyl Acetate	141-78-6	178	15	360	43900	7200	+610
Ethylene Glycol	107-21-1	2.51	41000	14000	NL	101.6	--
Formaldehyde	50-00-0	0.304	40	1.7	NL	12.3	--
Hydrazine	302-01-2	0.026	182	0.63	6.4	1.048	+610
Isobutyl Alcohol	78-83-1	18.7	120	300	4610	757.5	+610
Malathion	121-75-5	1.23	3.9×10^7	6.4×10^6	NL	50	--
Mercury	7439-97-6	0.00247	4.9×10^6	1600	NL	0.1	--
Methyl Isocynate	624-83-9	0.0287	2.5	0.013	7.1	1.17	+610
Nitric Acid (>70%)	7697-37-2	0.955	36	4.7	236	38.7	+610
Nitroglycerin	55-63-0	0.0494	5573	36	NL	2.0	--
Perchloroethylene	127-18-4	33.5	90	400	8270	1356	+610
Propionic Acid	79-09-4	1.12	235	35	276	45.5	+610
Toluene	108-88-3	27.9	45	165	6880	1131	+610
Xylene	1330-20-7	21.4	117	330	5280	868	+610

Note: Numbers for the evaporation time and quantity are rounded. Actual numbers used in determining the difference can be found in the appendices.

NL = Not Listed   NR = Not run (volume too small or parameters not in model)

REFERENCES

[ALOHA™ QA] "ALOHA™ Quality Assurance", Hazardous Materials Response and Assessment Division, National Oceanic and Atmospheric Administration, http://response.restoration.noaa.gov/cameo/alotech/quality.htm, (1998)

[Craig 95] Craig, D.K., J.S. Davis, R. DeVore, D.J. Hansen, A.J. Petrocchi, and T.J. Powell, "Alternative Guideline Limits for Chemicals without ERPGs", Amer. Ind. Hyg. Assoc. J. V.56, No.9, pp. 919-925 (1995)

[Craig 99] Craig, Douglas K.; "ERPGs and TEELs for Chemicals of Concern: Rev. 15 Abbreviated", Westinghouse Safety Management Solutions, Aiken SC, WSMS-SAE-99-00101, (January 1999)

[DOE 97] "Comprehensive Emergency Management System", Department of Energy , Washington D.C., DOE O 151.1, (Sept 1997)

[EMP 98] "Los Alamos National Laboratory Emergency Management Plan", Los Alamos National Laboratory, Los Alamos NM, LA-12900, Rev 1, (July 1998)

[EPA 87] "Technical Guidance for Hazardous Analysis: Emergency Planning for Extremely Hazardous Substances, U.S. Environmental Protection Agency, EPA-OSWER-88-0001, (December 1987)

[Evans, et al.] Evans, Mary; Jones, Robert; Overstreet, Roy, "Modeling Hydrochloric Acid Evaporation in ALOHA™", Modeling and Simulation Studies Branch, Hazardous Material Response and Assessment Division, Office of Ocean Resources Conservation and Assessment, NOAA, Seattle Washington, Report No. HAZMAT 93-3, (July 1993)

[Homann 96] Homann, Steven G., EPIcode® User's Guide, Homann Associates, Inc. Fremont, Ca, (1996)

[Lab Safety] Practices in the Laboratory: Handling and Disposal of Chemicals, National Academy of Sciences, National Academy Press, Washington DC, 1995

ATTACHMENTS

Attachment A – Physical Data as Modified from TEEL Listing (Rev 15)
Attachment B – Release Rate for the Liquids from TEEL Listing (Rev 15)
Attachment C – Quantity Limits for Liquids using Urban Terrain Dispersion
Attachment D – Quantity Limits for Liquids using Flat Terrain Dispersion